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**Motion of Aerosol Particles in Gas Following
Excitation by Resonance Radiation**

18410209b Moscow KOLLOIDNYY ZHURNAL in
Russian Vol 49, No 6, Nov-Dec 87 (manuscript received
28 Oct 85) pp 1125-1128

[Article by V.I. Roldugin, Institute of Physical Chemis-
try, USSR Academy of Sciences, Moscow]

[Abstract] A mathematical analysis was carried out on aerosol particle motion in a homogeneous gas due to excitation by the resonance radiation of a laser. Velocity distribution functions of excited and unexcited gas molecules were determined by a system of kinetic equations describing strong collisions [e.g., Ghiner, AV, et al., Phys. Lett., 96A(2): 79, 1983]. Actual velocities of the photophoretic movement were determined in a manner analogous to that used for calculating thermophoretic velocities [Deryagin, BV, and Bakanov, SP, Kolloid. Zhurn., 27(2): 377, 1959]. Particle motion was shown to be predicated on the asymmetry of the velocity distribution functions of the excited and unexcited molecules and on the fact that excited molecules are scattered differently by the surfaces of the particles than the unexcited molecules. The net effect is that the gas exerts a force on the particles, resulting in their motion relative to the center of the gas mass. Since the motion of the aerosol particles is fairly great, it can be readily measured with good accuracy. References 12: 10 Russian, 2 Western.

12172/9604

**Patterns of Liquid Dispersion in High Pressure
Ejectors**

18410220b Kiev KHIMICHESKAYA
TEKHNOLOGIYA in Russian No 6, Nov-Dec 87
(manuscript received 10 Feb 87) pp 43-46

[Article by Yu.P. Pavlenko, Ye.P. Pavlova, and I.G.
Reznichenko, Zaporozhye Industrial Institute]

[Abstract] Theoretical analysis of optimal jet opening angles, used in ejectors operating at high pressures, was conducted. Liquid dispersion could be achieved by centrifugal forces originating from stream rotation just before emerging from the nozzle, by an uneven profile of longitudinal velocity of the liquid propagation, turbulence, or cavitation. At high pressures, factors become important which are not significant at low pressures: for example, centrifugal forces have no effect on liquid dispersion. The most significant role is that of cavitation. This is the real reason for differences between the theoretically obtained values and those observed in practical runs. All factors must be considered in designing new equipment. References 4 (Russian).

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Preparation of N,N'-(7-thiaoctyl)urea: Sulfide Precursor of Diptocarpidine and Diptocarpiline Alkaloids

18410229b Tashkent KHIMIYA PRIRODNYKH
SOYEDINENIY in Russian No 5, Sep-Oct 87
(manuscript received 4 Feb 87) pp 742-744

[Article by O.V. Tolstikova, A.G. Tolstikov, and S.F. Aripova, Institute of Chemistry, Bashkir Branch, USSR Academy of Sciences, Ufa; Institute of Plant Substances Chemistry, Uzbek SSR Academy of Sciences, Tashkent]

[Abstract] Interest in sulfur-containing low molecular weight plant alkaloids from the biomedical viewpoint has included diptocarpiline and diptocarpidine, synthesized by the relatively rare *Diptychocarpus structus*

species. In view of the shortage of the raw material, a chemical approach was taken in the synthesis of N,N'-(7-thiaoctyl)urea, serving as a precursor to both agents. The synthetic approach consisted of the synthesis of 8-thia-nonanoic acid (I) by a reaction system involving 6-heptenoic acid, azobis(isobutyronitrile), and methyl mercaptan. The second step consisted of preparing the methyl ester of 8-thia-nonanoic acid (II) by the reaction of I with diazomethane. The next sequence involved the synthesis of 8-thia-nonanoic acid hydrazide (III) by the reaction of II with hydrazine hydrate. Finally, the reaction of III with concentrated HCl in ether with the temperature maintained at 10° C or lower resulted in the synthesis of N,N'-(7-thiaoctyl)urea in a 60% yield.

12172/9604

Effectiveness Criteria for Predesign Optimization of Chemical Technology

18410220c Kiev *KHIMICHESKAYA TEKHNLOGIYA*
in Russian No 6, Nov-Dec 87 (manuscript received
25 May 87) pp 56-61

[Article by A.I. Rozenfeld and G.Ye. Kanevets, Institute of Problems in Materials Technology, UkSSR Academy of Sciences, Kiev]

[Abstract] In planning and designing chemical processes, one often waits for data supporting the need for a given technology and its economic impact. Some of the indices of economic effectiveness are: cost effectiveness of the final product, capital investment, use of expensive, unavailable starting materials, etc. A special role is played by the quality of end products: in some cases this is the only criterion for acceptance or rejection of the material. Most of these concepts are difficult to handle a

priori. Criteria were developed which could be used in projecting optimization of chemical processes. They are: 1) criteria of economic effectiveness (minimal investment in starting materials and energy with maximization of the raw material processing index and energy utilization); 2) criteria for quality of production (minimal impurities in the end product and simplest procedures for reaching the desired product); 3) criteria of ecological preservation (minimum gaseous exhausts, minimum levels of noxious condensates), and 4) safety (fire, explosion, radioactivity, and toxic safety). Some of these criteria reinforce each other; some drive in opposite directions. Independent variables must be isolated which affect the overall optimization criterion. Two approaches to such optimization were proposed: additive combination of criteria and isolation of the main dominant criterion. References 7 (Russian).

7813/9604

Determination of Solubility of Perfluoroorganic Compounds in Water by Colloid Chemistry Methods

18410209a Moscow KOLLOIDNYY ZHURNAL in Russian Vol 49, No 6, Nov-Dec 87 (manuscript received 27 Sep 85) pp 1084-1089

[Article by Z.N. Markina, N.M. Zadymova, Ye.D. Shchukin, K.N. Makarov, and L.L. Gervits, Chemistry Faculty, Moscow State University]

[Abstract] Perfluoroorganic compounds have found extensive use in emulsions because of their low surface tension, and they are of considerable interest in medicine as blood substitutes in view of their capacity for gas transport. Because of their low solubility in water, special investigations were conducted on the determination of this parameter by means of a shift in the critical concentration for micelle formation and by assessment of the increment in the standard chemical potential ($\Delta\mu^\circ_{CF_2}$) for the transition of the perfluoromethylene radical from water at the water-perfluorocarbon interphase. In the former approach, evaluation of the effects of hydrophobic additives demonstrated that at 293 K, the solubility of perfluorodecalin and perfluorobutylamine stood at ca. 2×10^{-8} mol/l. Tensiometric studies showed that $\Delta\mu^\circ_{CF_2}$ was equal to -4.47 kJ/mol for perfluorononanoic acid at the perfluorodecalin boundary. On this basis, the solubilities in water of perfluorohexane, perfluoroheptane, perfluorooctane, perfluorodecalin, and perfluorododecane at 293 K were calculated to have the following respective values: 9×10^{-4} , 1.45×10^{-4} , 2.3×10^{-5} , 5.8×10^{-7} , and 1.5×10^{-8} mol/l. Figures 2; references 16: 12 Russian, 4 Western.

12172/9604

Determination of Refractive Index of Pigments with Unknown Microstructure from Light Scattering

18410209c Moscow KOLLOIDNYY ZHURNAL in Russian Vol 49, No 6, Nov-Dec 87 (manuscript received 11 May 85) pp 1175-1178

[Article by D.A. Ashkinadze, I.M. Radyuk, and A.P. Shavel, Belorussian University; Scientific Research Institute of Applied Physical Problems, Minsk]

[Abstract] The requirements for large samples in assessment of the overall index of refraction ($m = n - i\kappa$) of fine pigment suspensions by means of reflective spectroscopy renders such methods essentially inapplicable to the type of fine organic pigment suspensions used in paints.

Consequently, in order to avoid difficult physical determinations of microstructural parameters, n and κ were determined from light scattering, using the gamma function to describe the distribution of the suspended particles. The angular dispersion factor and the quenching factor were obtained by applying the Mie equation for a single scattering with $0.63 \mu\text{m}$ light and multiple scattering with high flux illumination. This approach to the determination of optical coefficients, based on the calculation of n , κ , and r (r = modal radius of particles) from the attenuation and directed light scattering factors in the 20° [is less than or equal to] β [is less than or equal to] 90° angle range, was ascertained to be a workable solution with an acceptable accuracy. Figures 1; references 15: 14 Russian, 1 Western.

12172/9604

Electric Properties of Aqueous Suspensions of Synthetic Diamond

18410220a Kiev KHIMICHESKAYA TEKHOLOGIYA in Russian No 6, Nov-Dec 87 (manuscript received 14 Jul 86) pp 26-29

[Article by L.I. Tertykh, Institute of Colloid Chemistry and Water Chemistry, UkSSR Academy of Sciences, Kiev]

[Abstract] Electric properties of aqueous dispersions of synthetic diamond were studied. The investigation included the effect of the chemical nature and concentration of electrolytes on specific electroconductivity, electrophoretic mobility, and electrokinetic potential. A flat quartz glass container equipped with platinum electrodes was filled with an aqueous suspension of diamond powder. Electrophoretic mobility was visually registered in an optical microscope. Particle size was determined with an electron microscope. Mechanically produced diamond particles formed conglomerates which broke down into individual particles upon exposure to ultrasound; after several days, the aggregates formed again. The chemical nature and electrolyte concentration had a definite effect on electrophoretic mobility: mono- and divalent cation-containing electrolytes lowered the ξ -potential of negatively charged diamond particles, while electrolytes with three and four valent cations led to their recharging. Thus, results have shown that the ability to alter the electrokinetic potential of dispersions makes it possible to prepare composition plating from diamond and polymers either at the anode or cathode. Figures 3; references 7: 6 Russian, 1 Western.

7813/9604

Initiation of Detonation Processes in Model Oxidizer-Fuel Mixtures

18410219a Moscow *KHIMICHESKAYA FIZIKA*
in Russian Vol 6, No 11, Nov 87 (manuscript received
15 Jan 87) pp 1507-1510

[Article by V.F. Martynyuk, A.A. Sulimov, M.K. Sukoyan, and A.I. Melkumov, Institute of Chemical Physics, USSR Academy of Sciences, Moscow]

[Abstract] Critical conditions were studied for initiation of detonation processes in model mixtures containing ammonium perchlorate (APC) and polymethyl methacrylate at different ratios, while varying charge density over a wide range. It was shown that in areas of low charge density, addition of fuel to the oxidizer lowers the critical pressure of detonation initiation, indicating the existence of an interaction between components during initiation of the detonation. In the high charge density region, where the detonation rate does not depend on the density-to-component ratio, the P_{cr} values of the mixtures studied were similar, indicating the determining role of the APC breakdown reaction in initiating detonation. In the intermediate areas where detonation velocity drops with an increase in density, in the initiation pressure range P_{min} [is less than or equal to] P [is less than or equal to] P_{cr} , nonstationary low velocity modes are observed, emanating from stages of the heat production process during charge detonation. References 10: 8 Russian, 2 Western.

7813/9604

Feasibility of Conducting Chemical Reactions in High Dynamic Pressure Zones

18410219c Moscow *KHIMICHESKAYA FIZIKA*
in Russian Vol 6, No 11, Nov 87 (manuscript received
17 Jan 87) pp 1576-1582

[Article by S.S. Batsanov, All-Union Scientific Research Institute of Engineering Physics and Radio Engineering Measurements, Mendeleyevo]

[Abstract] A number of papers have appeared, showing that reactions could occur in a 10^{-5} to 10^{-6} s time frame in zones of high dynamic pressures. In the present work,

an attempt was made to analyze critically these publications. It was concluded that hetero- and solid phase reactions could be conducted in a period of 10^{-6} to 10^{-5} s under conditions of explosive compression. These ultrahigh diffusion rates are due to high temperature and low activation energies in the case of heterophase reactions and due to a difference of mass velocities of the mixture components, resulting in forced diffusion on the order of $\Delta \mu$ in solid phase reactions. Hence, depending on the setup of the experiment and properties of the components, reactions could be conducted in the high pressure zones or in the discharged state. References 59: 39 Russian, 20 Western (3 by Russian authors).

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Self-Ignition of $NF_2-H_2O_2$ Mixture at 300-615 K

18410219d Moscow *KHIMICHESKAYA FIZIKA*
in Russian Vol 6, No 11, Nov 87 (manuscript received
30 Jan 87) pp 1590-1591

[Article by V.B. Rozenshteyn and Yu.R. Bedzhanyan, Institute of Chemical Physics, USSR Academy of Sciences, Moscow]

[Abstract] In previous work, a chain reaction mechanism was shown for the reaction of $NF_2 + H_2O_2$ at 300 K. In this work, this reaction was studied at temperatures exceeding 300 K under stream flow, using a combined EPR/LMR spectrometer. On the basis of the fact that component reaction rates were not temperature dependent, it was concluded that indeed the chain mechanism prevails even at temperatures exceeding 300 K (up to 615 K). The position of the concentration limit of NF_2 was determined as a function of temperature. The chain development rate constant was determined $K_{HQ2 + NF2} = 2.3 \cdot 10^{-11} \exp[650 \text{ [plus or minus] } 250/T] \text{ cm}^3/\text{s}$. This finding could be used in promoting complex chemical processes in which the limiting step is the HO_2 reaction. References 9 (Russian).

7813/9604

Prospects for Development of Inorganic Chemistry in Ukrainian SSR in 12th Five Year Plan
18410154 Kiev VISNYK AKADEMIYI NAUK
UKRAYINSKOYI RSR in Ukrainian No 10, Oct 87
pp 86-87

[Article by I.A. Sheka, corresponding member, UkrSSR Academy of Sciences, and Ye.Yu. Kriss and Yu.A. Maletin, candidates of chemical sciences]

[Text] In May 1987, the UkSSR Section on Inorganic Chemistry of the Scientific Council of the USSR Academy of Sciences held its extramural session at the Physical Chemistry Institute imeni O.V. Bogatskiy of the UkSSR Academy of Sciences (UAS). The session was attended by more than 50 scientists and chiefs of various institutions of the UAS, departmental institutes, and heads of educational institutions in Kiev, Odessa, Kharkov, Dnepropetrovsk, Donetsk, Lvov, Voroshilovgrad, Simferopol, Zaporozhye, and other cities.

I.A. Sheka, corresponding member of the UAS and head of the Scientific Council of the UAS, addressed some of the more fundamental problems affecting the development of inorganic chemistry in the Ukraine in light of restructuring as it impacts on chemistry. The participants were greeted by S.A. Andronati, director of the Institute and corresponding member of the UAS, who also covered scientific achievements at the Institute and plans for inorganic chemistry at the Institute in the future.

A number of reports were read, dealing with various current problems in inorganic chemistry at the different scientific centers in the Ukraine. K.B. Yatsymirskiy, Academician of the UAS, reported on coordination compounds between metals and peptides, and V.V. Strelko, doctor of chemical sciences, covered second generation inorganic sorbents. N.P. Yefryushyna, doctor of chemical sciences, dealt with luminophors derived from simple and mixed borates of periodic table group II and III elements. Finally, Doctor of Chemical Sciences H.L. Kamalov called attention to molecular mechanics as an approach to studies on coordination compounds.

The participants also discussed the papers presented by candidates of chemical sciences S.B. Meshkova (Correlation of the Properties of Lanthanides with the Quantum Mechanical Characteristics of their Ions), Yu.A. Maletin (Electron Transfer Reactions Accompanying Coordinational Restructuring in Complexes), H.D. Zegzhda (Synthesis and Redox Transformations of Metal Complexes in Thiol-Disulfide Systems), and O.M. Fedorenko (Computers and Practical Aspects of the Solubility Method). These papers were presented as doctoral dissertations. The basic trends expressed in these presentations were approved and complemented by critiques intended to bring these studies to successful completion.

Reports were also presented by the heads of scientific collectives about studies completed in 1986 and plans for 1987. In addition, the report of the Scientific Council, covering 1986, was also considered, as were plans for scientific and administrative projects in 1987.

In comparison with previous years, research on inorganic compounds has gained considerable prominence in the Ukraine, with considerable attention accorded to solid phase studies based on new physical methods and theoretical advances. However, it has been noted that not all the research projects have reached the stage of practical application. Ukrainian inorganic chemists have not received sufficient support from the ministries and departments which stand to benefit from their work.

Research conducted at the Physical Chemistry Institute and other scientific establishments of the UAS in Odessa was evaluated in positive terms. The various projects dealt with development of waste-free technologies, new inorganic materials for use as luminophors, and studies on organometallic ligand complexes useful in analytical chemistry and as catalysts and vulcanization accelerators.

The session approved the following as priority items for the Ukraine in the 12th Five-Year Plan: synthesis of novel inorganic compounds and materials with desirable physicochemical characteristics, based on phosphides, oxides, fluorides (chalcogenides), phosphates of special carbon and inorganic sorbents, etc. In addition, new emphasis has to be placed on inorganic synthesis, especially methods relying on laser, plasma, and self-propagating high-temperature syntheses and sol-gel technologies; the following are examples:

—development of solid state chemistry and crystal chemistry, development of the theory of solid state synthesis of metallic and nonmetallic compounds and the technologies involved in their production, and development of means for preparing various films on various substrates;

—synthesis and evaluation of new types of coordination compounds, including macroligands, with potential use in lasers, fiber optics, electrochemistry, polyfunctional additives, etc.;

—development of new technologies for processing low-quality aluminum and lithium ores, as well as secondary raw materials pertaining to nonferrous, rare, and noble metals. Methods should be developed for the isolation and purification of industrial products, based on fundamental assessments of chemical processes, as well as for the purification of industrial solvents. Nondestructive methods must also be developed for monitoring superficial and serious defects in commercial products; and

—development of biocoordination chemistry, involving the modeling of vital processes in which coordination compounds participate, evaluation of the role of trace

metals in these processes, decontamination of the environment, and the creation of novel therapeutic agents and chemical agents for the protection of plants and animals.

Another decision reached at the session was to maintain the functional form of the Scientific Council of the UAS in relation to inorganic chemistry and to hold seminars on inorganic chemistry at least on an annual basis. Finally, reports of the heads of theoretical seminars are to be presented on a systematic basis.

The session also dealt with the activities of the editorial board of UKRAINSKIY KHMICHESKIY ZHURNAL.

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12172/9604

Recrystallization of Oceanic Ferromanganese Nodules

18410208c Kiev DOKLADY AKADEMII NAUK UKRAINSKOY SSR: SERIYA B in Russian No 10, Oct 87 (manuscript received 30 Mar 87) pp 42-45

[Article by I.M. Obushchenko, F.D. Ovcharenko, Academician, UkSSR Academy of Sciences, N.V. Pertsov, and N.M. Topkina, Department of Natural Dispersed Systems, Institute of Water Chemistry and Colloid Chemistry, UkSSR Academy of Sciences, Kiev]

[Abstract] Studies were conducted on the crystallization process in ferromanganese nodules obtained from the Indian and Pacific oceans, which were analyzed to consist of the following five fundamental forms (in wt.%): MnO — 28.0/26.0, Fe₂O₃ — 14.2/19.5, Co — 0.07/0.82, Ni — 0.08/0.24, and Cu — 0.03/0.58. The milled nodules were graded on 0.40 to 0.05 mm sieves, then subjected to 3-5 h annealing at 1273 K in air, as well as to recrystallization for 5 h in H₂SO₄, Na₂SO₄, NaOH, and Na₂CO₃ at the corresponding boiling points under atmospheric pressure at 473 K. In addition, recrystallization was also conducted in NaNO₃, NaPO₃, and KCl melts for 3-5 h at 613, 923, and 1073 K, respectively. Studies of the original and recrystallized samples by X-ray phase analysis showed that hydrothermal treatment led to the formation of aluminosilicates (Na₂O·Al₂O₃·3.3-3.5SiO₂·4.3-5.7H₂O). Crystallization proceeded much more rapidly with the Indian Ocean nodules than those obtained from the Pacific, presumably due to the fact that the level of aluminosilicates was much lower in the original Pacific nodules than in the

Indian samples. Recrystallization from melts of inorganic salts and in annealing at 1273 K involved the manganese and iron oxides: Mn₂O₃, MnO₂, α -Fe₂O₃, and γ -Fe₂O₃. These findings indicate that the development of crystalline nodules requires more extreme thermal and chemical conditions than are commonly encountered in the deep sea. Figures 2; references 11: 7 Russian, 1 Polish, 3 Western.

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Laser Effects on Electrophysical Behavior of Solid Mg_xCd_{1-x}Te Solutions

18410213a Moscow POVERKHNOST: FIZIKA, KHIMIYA, MEKHANIKA in Russian No 12, Dec 87 (manuscript received 2 Mar 87) pp 106-111

[Article by P.A. Akhoyan, A. Baydullayeva, N.Ye. Korsunskaya, P.Ye. Mozol, I.Ya. Gorodetskiy, G. Garyagdyev, and O. Nuryagdyev, Institute of Semiconductors, Ukrainian SSR Academy of Sciences, Kiev]

[Abstract] Solid Mg_xCd_{1-x}Te (I) solutions represent poorly studied A^{II}B^{VI}-type compounds with photo- and electroluminescent properties, suggesting their potential application in light-emitting diodes. In view of this, the effects of pulsed (2×10^{-8} s) ruby laser light on I were evaluated for their impact on the electrophysical behavior of single I crystals. Studies were conducted with crystals displaying n-type conductivity being subjected to laser intensities below the threshold intensity (I_t), leading to destruction and melting. Examination of the relationship between the number of impulses (N) and equilibrium and photoconductivities at intensities below I_t revealed two types of crystals. Crystals in one category showed an initial increase in equilibrium conductivity as well as photoconductivity, reaching a maximum plateau (in analogy to CdS, CdSe, and Zn_xCd_{1-x}Se). The other type responded with much higher increases in equilibrium and photoconductivities; after reaching a maximum value, a further increase in N induced periodic oscillations in the conductivity patterns. In the latter case, the effects were attributed to the formation of a conductive Te surface film, with the oscillations being abrogated by washing with 1 N KOH in methanol and with HCl to remove oxides. Washing the former class of crystals had no effect on the findings. The laser-induced appearance of residual conductivity and increased equilibrium conductivity was attributed to an increase in the concentration of shallow hydrogen-like donors with E_d = 0.015 eV (probably due to formation of Cd_i) and formation of deep donors with E_d = 0.035 eV (attributed to v_{Te} vacancies). Figures 4; references 19: 11 Russian, 8 Western.

12172/9604

Reactions of 4-methyl-7-diethylaminocoumarin with Electrophilic Reagents

18410205a Riga KHIMIYA

GETEROTSIKLICHESKIKH SOYEDINENIY in

Russian No 10, Oct 87 (manuscript received 20 Jun 86)
pp 1324-1332

[Article by M.A. Kirpichenok, S.L. Levchenko, and I.I. Grandberg, Moscow Agricultural Academy imeni K.A. Timiryazev]

[Abstract] In view of the importance of 7-aminocoumarins as laser dyes, studies on this class of compounds were expanded by the reaction of 4-methyl-7-diethylaminocoumarin (I) with various electrophilic reagents. A series of 3-, 6-, and 8-substituted derivatives were prepared by the reaction of I with acetic anhydride, styrene, dihydropyrene, phenylacetylene, Lewis acids, and copper (II) halides, using sulfuric acid, aluminum chloride, or titanium tetrachlorides as catalysts. In general, the electronic spectra of the resultant 7-aminocoumarins showed a hypsochromic shift in relation to the electron donor properties of substituent groups at position 3. The characteristic feature of I is a tendency toward charge separation within the molecule. While the amino group can stabilize a positive charge, maximum electron density is localized on the exocyclic oxygen atom and the C₁₃ atom of the pyrone ring. The polarization is also supported by NMR data, indicating strong p- π coupling in the nitrogen atom-oxygen atom system of the carbonyl group. Charge separation in 7-aminocoumarin has the practical significance that these compounds may serve as electron donors. An effective method for the introduction of Cl or Br into position 3 consisted of the reaction of I with Cu(II) halides in nitromethane and boiling for 15 h. References 14: 8 Russian, 6 Western.

12172/9604

Inelastic Interaction of Fluorine Molecules with Secondary Electrons Formed in Initiation of Chemical Hydrogen Fluoride Lasers by Rapid Electron Beams

18410206a Moscow KHIMIYA VYSOKIKH ENERGIY in Russian Vol 21, No 6, Nov-Dec 87 (manuscript received 23 Dec 85) pp 539-543

[Article by V.V. Braslavets, P.K. Buletsa, V.N. Slavnik, P.V. Feltsman, and A.S. Bashkin, Uzhgorod State University; Physics Institute imeni P.N. Lebedev, USSR Academy of Sciences]

[Abstract] A study was conducted on the dissociation of fluorine molecules by slow electrons since it has been shown that initiation of chemical H₂-F₂ lasers can be

conveniently achieved with relativistic electrons. Ionization of the fluorine molecule by a relativistic electron (e_r) leads to the formation of a slow secondary electron (e_s) with energies in the ca. 30 to 35 eV range: F₂ + e_r [leads to] F₂⁺ + e_r + e_s. One e_s leads to the appearance of a large number of e₀, which react with molecular fluorine to form fluorine atoms. Assessment of single collision events with the slow electrons in the 0.5-30 eV range, i.e., monochromatic in terms of energy, resulted in identification of each of the following basic reactions: F₂ + e [leads to] F + F + e; F₂ + e [leads to] F + F; F₂ + e [leads to] F⁺ + F + 2e; and F₂ + e [leads to] F + F⁺ + e. Evaluation of the effects on fluorine molecules in terms of electron energy showed that the dissociation cross-section of the fluorine molecules was, for example, $\delta = 7 \times 10^{-17}$ cm² with 10 eV electrons. Dissociation of the fluorine molecules into atoms was the primary process of inelastic collisions in the 4-20 eV range. Kinetic studies of this type may be used in assessing the mechanisms of initiation of H₂-F₂ lasers with electrons. Figures 4; references 17: 6 Russian, 11 Western.

12172/9604

Effects of Substituents on Light Fastness of Imitrine Laser Dyes

18410208a Kiev UKRAINSKIY KHIMICHESKIY ZHURNAL in Russian Vol 53, No 11, Nov 87 (manuscript received 8 Apr 86) pp 1197-1200

[Article by L.T. Chertorizhskaya, V.P. Kruglenko, A.A. Timoshin, M.V. Povstyanoy, and Ya.N. Malkin, Kherison Industrial Institute]

[Abstract] To assess the light fastness of imitrine dyes (imidazo[1,2-b]-1,2,4-triazine) that have potential laser applications, the effects of illumination with mercury lamps DRT-375 and DRSh-1000 were quantified in relation to substituents on both rings (R = Ph, H, Cl, CH₃, or C₃H₇). Analysis was conducted in terms of spectrophotometric measurements of the optical densities at 420-440 nm in ethanol. Rate constants were calculated from the rate of bleaching of the different compounds in relation to the intensities of the lamps. The data showed that the effects of the various substituents were interdependent and that more detailed studies will have to be conducted to assess their suitability for use in lasers. Analysis of fluorescence spectra in toluene and triplet-triplet absorption 10⁻³ s after excitation showed that, in the presence of oxygen, photodecomposition of the imitrines was reduced three-fold. However, there were no oxygen effects on photodecomposition in ethanol. Since the triplet state is completely quenched by oxygen, it appears that irreversible light-induced degradation of imitrines proceeds via the lowest triplet state. Figures 2; references 6 (Russian).

12172/9604

Magnetic and Structural Characteristics of Mesophase-Forming Single Crystals of Copper Complexes with Schiff Bases

18410228a Novosibirsk ZHURNAL STRUKTURNOY
KHIMII in Russian Vol 28, No 5, Sep-Oct 87
(manuscript received 9 Apr 86) pp 157-158

[Article by I.G. Bikchantayev, A.P. Polishchuk, and I.V. Ovchinnikov, Kazan Engineering Physics Institute]

[Abstract] EPR and X-ray structural studies were conducted on single crystals of complexes formed by copper and Schiff bases, compounds demonstrated to form a mesophase. The present study concerned complexes of the following type: $[C_7H_{15}O-C_6H_3(O)CH=N-C_6H_4R]_2Cu(II)$, with $R = OC_4H_9$. The single crystals fell into the C2/c monoclinic system, with unit cells

characterized by $a = 43.662$ Angstroms, $b = 10.267$ Angstroms, $c = 18.506$ Angstroms, $\beta = 107.29^\circ$, and $Z = 8$. The crystals melted at $132.9^\circ C$ with the formation of a smectic-type mesophase, showing a typical isotropic melt above $140^\circ C$. The isotropic melt consisted only of planar complexes, giving a single line on the spectrum with $g = ca. 2.089$. EPR spectra of the mesophase showed two independent lines with g factors that were quite close to those obtained for the planar and tetrahedral complexes of the single crystals. The EPR data were interpreted to signify that the magnetic interactions between molecules within a layer were much stronger than between layers. Thus, the single crystals possess a two-dimensional magnetic system. Figures 2; references 5: 2 Russian, 3 Western.

12172/9604

Synthesis and Herbicide Activity of N-Methylcarbamoyl Derivatives of 2-Hydroxyethyl Esters of 2,4-Dichlorophenoxyalkylcarboxylic Acids
18410205c Baku DOKLADY AKADEMII NAUK AZERBAJDZHANSKOY SSR in Russian No 10, Oct 87 (manuscript received 21 May 86) pp 38-41

[Article by D.N. Khydyrov, A.K. Arabov, N.V. Lipushkina, M.M. Gasanova, and R.A. Babakhanov, corresponding member, AzSSR Academy of Sciences, AMI [expansion unknown] imeni N. Narimanov]

[Abstract] In view of the herbicide activities of many 2,4-dichlorophenoxy-carboxylic acids (I), novel N-methylcarbamoyl derivatives of 2-hydroxyethyl esters of I were synthesized and tested for similar activities. Reaction of I with methyl isocyanate at 45-50° C with catalytic quantities of triethylamine resulted in the synthesis of previously undescribed N-methyl carbamates of β -hydroxyethyl 2,4-dichlorophenoxy cetate and of β -hydroxyethyl α -2,4-dichlorophenoxybutyrate. Both compounds evidenced herbicide activities against dicotyledonous weeds, but not against monocotyledons. References 8: 7 Russian, 1 Western.

12172/9604

Benzoylation of 2,2,4-Trimethyl-1,2-Dihydroquinoline Dimer
18410206b Ivanovo IZVESTIYA VYSSHIKH UCHEBNYKH ZAVEDENIY: KHIMIYA I KHIMICHESKAYA TEKHOLOGIYA in Russian Vol 30, No 10, Oct 87 (manuscript received 18 Nov 86) pp 23-28

[Article by Zh.V. Shmyreva and Kh.S. Shikhaliyev, Chair of Organic Chemistry, Voronezh State University imeni Lenin's Vomsomol]

[Abstract] The demonstration that acylated derivatives of 2,2,4-trimethyl-1,2-dihydroquinoline (I) are effective fungicides led to synthesis of further derivatives for biological testing. In the present study, compounds with potential biological activity were produced by benzoylation of I and hydrogenated I (II). Data are presented on the reaction of I and II with benzoyl chloride under different conditions to synthesize the mono- and dibenzoyl derivatives of the dimers. Data on the products are summarized in tabular form, containing information on the melting points, empirical formulas, yields, and IR spectra. References 6: 3 Russian, 3 Western.

12172/9604

Economic Incentives within Self-Financing Framework

18410213c Moscow *KHIMIYA I TEKHNLOGIYA TOPLIV I MASEL* in Russian No 11, Nov 87 pp 7-10

[Article by G.V. Zhuk, chief, Financial Administration, USSR Ministry of Petrochemical Industry]

[Abstract] With the implementation of self-financing in Soviet industry, special emphasis has to be placed on financial incentives for workers. In the USSR Ministry of the Petrochemical Industry, efforts have been made to make workers aware of the interrelationship between the financial health of their factory or plant and their wages and the manner in which the former depends on their productivity. To a large extent, such considerations are also based on the quality of production. In the latter case, there is considerable involvement of skilled specialists and scientists, whose motivation and interest must also be taken into consideration by management. Considerable leeway has been granted to the individual industries in recognizing these factors and in determining policies best suited to meeting their quality and job satisfaction goals in conjunction with high productivity.

12172/9604

Quality Improvement and Standardization of Aviation Gasolines

18410213d Moscow *KHIMIYA I TEKHNLOGIYA TOPLIV I MASEL* in Russian No 11, Nov 87 pp 39-40

[Article by Ye.A. Nikitina, V.Ye. Yemelyanov, P.V. Chulkov, N.I. Cherkasova, and S.R. Lebedev, All-Union Scientific Research Institute of Petroleum Refining]

[Abstract] Global production of aviation gasoline stands currently at 0.1% of total aviation fuel production. In the USSR, the number of brands has been reduced to two — B-91/115 and B-95/130 — with production of the latter accounting for only 6.7% of the total output. Plans are currently under way for production of a single brand based on B-91/115 for both airplanes and helicopters. In following the practices abroad, the new aviation gasoline (B-92) will contain no more than 2 g/kg of tetraethyl lead and have a minimum octane number of 91.5 and a specific heat of combustion of 42,737 kJ/kg. The reduction in tetraethyl lead will also reduce the concentration of antioxidants required for stability and enable the use of 0.01% or less of ionol along with p-hydroxydiphenylamine. The cost effectiveness of the new type of aviation gasoline, once it goes into production, is expected to reach 9.5 million rubles per year. References 6: 1 Russian, 5 Western.

12172/9604

Thermoelectrooptical Memory Effects in Smectic Type A Liquid Crystals

18410203b Baku DOKLADY AKADEMII NAUK
AZERBYADZHANSKOY SSR in Russian Vol 43,
No 1, Jan 87 (manuscript received 9 Aug 85) pp 29-33

[Article by A.A. Abbas-Zade and V.I. Khatayevich, Scientific Production Association of Space Research]

[Abstract] Smectic liquid crystals are capable of relatively long retention of textural changes induced by outside forces, displaying in that sense a type of optical memory. Such liquid crystals may be used as large-capacity, controlled-memory storage devices. Reversible memory in smectic type A crystals is dependent on transition from a transparent isotropic state to a diffracting confocal medium. Transition to the isotropic state may be induced by electrohydrodynamic instability or the application of heat. Another form of thermoelectrooptical retention of memory in smectic type A liquid crystals is based on regulation of induced double refraction. Studies with two liquid crystals with Δn [is greater than] 0 — $C_6H_5O-benz-COO-benz-NO_2$ and $C_6H_5-benz-benz-CN$ — of the threshold and temporal characteristics of confocal-isotropic transitions demonstrated that thermoelectrooptical recordings can occur directly in the smectic type A phase. In addition, the studies also showed structural changes due to thermoelectrooptical influences in transition from the nematic to the smectic type A phase. The advantages offered by controlled application of double refraction rest on the fact that much weaker controlling potentials are required as well as much shorter recording times. In addition, the interference color in the 1.6 to 6 V range is easily controlled, as is the contrast at 6 V that approached a ratio of 200:1. Figures 3; references 14; 6 Russian, 8 Western.

12172/9604

Solvent Effects in Electroinitiated Copolymerization of Phenyl Isocyanate and Methyl Methacrylate in Presence of Carbon Fibers

18410208b Kiev UKRAINSKIY KHIMICHESKIY
ZHURNAL in Russian Vol 53, No 11, Nov 87
(manuscript received 6 Jan 86) pp 1209-1213

[Article by V.G. Matyushova, T.E. Lipatova, and T.S. Khramova, Institute of Chemistry of High Molecular Weight Compounds, UkSSR Academy of Sciences, Kiev]

[Abstract] An assessment was made of solvent effects on electrically initiated copolymerization of phenyl isocyanate and methyl methacrylate in acetonitrile and dimethyl acetamide, two solvents with similar dielectric constants but different solvating capacities. Carbon fibers served as the cathode component in the system. Spectroscopic, chemical, and electrochemical studies demonstrated that the solvent exerted a profound effect

on the yield and composition of the products. Conductivity of the methacrylate and isocyanate in acetonitrile and acetamide was, respectively, 6.23×10^{-3} and $2.27 \times 10^{-3} \text{ ohm}^{-1} \text{ cm}^{-1}$, with the electronic spectra of the anion radical in both solvents indicating a higher degree of solvation in dimethyl acetamide. Furthermore, the yield of electrolytic products in acetonitrile was on the order of ca. 80-90% and was virtually unaffected by the current employed, whereas in dimethyl acetamide, the maximum yield was 50% and diminished to 12% as the current increased from 1 to 6 mA/m². In addition, the copolymer isolated from acetonitrile by diethyl ether precipitation was enriched in phenyl isocyanate, whereas the m/n ratio for the copolymer isolated from dimethyl acetamide was close to 2 regardless of the current density. Figures 3; references 11; 6 Russian, 5 Western.

12172/9604

Enhancement of Hydrodynamic Stability of Polyacrylamide

18410208d Kiev DOKLADY AKADEMII NAUK
UKRAINSKOY SSR: SERIYA B in Russian
No 10, Oct 87 (manuscript received 22 Jun 86) pp 51-54

[Article by I.L. Povkh, corresponding member, UkSSR Academy of Sciences, T.V. Stupnikova, T.V. Vyshkina, and B.P. Makogon, Donetsk State University]

[Abstract] This study was concerned with the enhancement of hydrodynamic stability of polyacrylamide by the addition of agents capable of storing or capturing energy and then dissipating it without affecting the structure or conformation of the macromolecule. Rheologic studies conducted on polyacrylamide, modified by the addition of arginine, showed that formation of polyacrylamide-arginine complexes prevented deterioration of the polymer. Complexing was attributed to hydrogen bond formation between arginine and the $-C=O$ and $-NH_2$ groups on the polyacrylamide. The protective effects were attributed to the efficiency of the arginine group in capturing energy and dissipating it as a result of tautomer transformations. Other amino acids — such as glycine and leucine — also formed complexes with polyacrylamide but failed to protect the polymer from damage since they do not possess double bonds and do not act as energy traps. Furthermore, thymine and adenine, although capable of functioning as energy traps, failed to protect polyacrylamide since complexing with polyacrylamide did not take place. These observations demonstrated that effective agents need to form complexes with polyacrylamide and act as energy traps. Figures 2; references 10; 9 Russian, 1 Western.

12172/9604

Effects of Heat Treatment and High Humidity on Conductivity of Metallized Nitron Fibers

18410218a Moscow KHIMICHESKIYE VOLOKNA in Russian No 6, Nov-Dec 87 (manuscript received 18 Dec 86) pp 12-14

[Article by D.N. Akbarov, G.F. Vlasenko, A.K. Yenikeyeva, O.Yu. Mikhaylova, L.A. Samoylova, and T.N. Ovchinnikova]

[Abstract] Studies with metallized nitron fibers have demonstrated that drying conditions have a marked effect on the electrical characteristics of such products. The best protection against extensive oxidation of the nickel coat was obtained by drying in the temperature range 120-140° C for 30 min. with removal of the water lost by evaporation, an approach that was equally effective in the case of chemically-metallized fibers, as well as those in which chemical metallization was followed by galvanic metallization. Greater electrophysical stability was demonstrated by the latter class of fibers (up to 12 wt.% Ni), with resistivities in the 3.6 to 3.9×10^{-5} ohm m range. The resistivity of fibers metallized only by chemical means (ca. 7 wt.% Ni) was on the order of 2.8 to 3.2×10^{-4} ohm m. Figures 2; references 3 (Russian).

12172/9604

Relationship Between Viscoelastic Properties of "Nucleus-Membrane"-Type Fibers and Drawn Fiber Products

18410218b Moscow KHIMICHESKIYE VOLOKNA in Russian No 6, Nov-Dec 87 (manuscript received 18 Mar 87) pp 20-22

[Article by V.P. Kostromin, N.B. Buleva, S.N. Kolomiets, and V.M. Levin]

[Abstract] Extensive utilization of combined extrusion technology for the production of lamellar films and bicomponent fibers led to an assessment of the viscoelastic properties of the polystyrene (PS) and polymethacrylate (PMC) components with respect to the end product. Evaluation of the viscosities over 200-260° C showed that the energy of activation for the flow of PS was 96 kJ/mol, and for PMA 141 kJ/mol. However, the effects of the shear rate on the effective viscosity were much more pronounced in the case of PS than in PMC. Thus, both factors favored the formation of bicomponent fibers with variable viscosities of the polymers in the nucleus and the sheath. Tabulated data are presented for different geometries of fiber-drawing machines, including the spinnerette element, leading to the demonstration that, depending on the shear stress in the spinnerette, the temperature, and the rate of extrusion, "nucleus-membrane" type fibers may be produced with

variable viscosities of the components. The latter constitute an important characteristic of optical fiber polymers. An increase in the rate of extrusion above that recommended for a given ratio of the viscosities of the two components will lead to disruption of the membrane with retention of nuclear patency and of the fiber as a whole. Such events are responsible for the low light-transmission of polymer optical fibers. Figures 2; reference 1 (Russian).

12172/9604

Effects of Lasers on Fibers: Fundamental Stages and Threshold Effects

18410218c Moscow KHIMICHESKIYE VOLOKNA in Russian No 6, Nov-Dec 87 (manuscript received 23 Apr 87) pp 42-44

[Article by B.A. Vinogradov and K.Ye. Boyarkin]

[Abstract] The effects of a CO₂ laser on natural and synthetic fibers were studied by thermal and spectral analyses, as well as by a photoacoustic (PA) method. The PA method was based on changes in the PA signal due to periodic thermal expansion of the fibers and the adjacent gas layer (air or helium), which led to deviation of the intensity (I) of the PA signal from linearity when plotted against the flux density of the laser (q_0). Plots of the I of PA generated by fibers exposed to the laser against q_0 in the case of aramid PM and aramid PAA (polyamido acid, noncyclic) showed deviation from linearity at a certain q_0 range, corresponding to fiber destruction by the CO₂ laser. The initial linear portion of the plot corresponded to thermoelastic oscillations in the fibers and heat transfer to the surrounding gas. The point of transition from linearity to deviation was designated the proportionality threshold (q_{pt}). Analysis of the data demonstrated that the nonlinear portion of the plot corresponded to endothermic processes, which were more pronounced in the case of aramid PAA than for aramid PM, due to loss of physically and chemically bound water. IR and X-ray spectroscopies confirmed the occurrence of chemical and supramolecular changes in the fibers, with virtually 100% imidization of the noncyclic fragments and condensation of the fibers. For aramid PM, these changes occurred in the q_0 range of 15 to 30 W/cm², and for aramid PAA, in the 12 to 34 W/cm² range. On the basis of the q_{pt} value and the thermoelasticity constant K_{te} ($= \Delta I / \Delta q_0$), the various fibers were divided into three categories. Aramid and polyamidebenzimidazole fibers were characterized by q_{pt} values ranging from 9.0 to 14.0 W/cm² and K_{te} in the 1.5 to 3.0 W⁻¹ cm² range. Another group was represented by lavsan, kapron, and nitron with $q_{pt} = 3.0$ -7.0 W/cm² and $K_{te} = 0$ -0.4 W⁻¹ cm². Finally, a third group was represented by cellulose fibers, silk, and fur hairs with $q_{pt} = 3.0$ -7.0 W/cm² and $K_{te} = 0.5$ to 1.5 W⁻¹ cm². Figures 2; references 5; 3 Russian, 2 Western.

12172/9604

Investigation of Uranium (IV) Reaction with Xenon Difluoride by Chemiluminescence, Spectrophotometry, and Spectrofluorometry Methods

18410217a Leningrad RADIOKHIMIYA in Russian Vol 29, No 6, Nov-Dec 87 (manuscript received 26 Aug 86, after final revision 29 May 87) pp 741-745

[Article by A.V. Mamykin and V.P. Kazakov]

[Abstract] Chemiluminescence (CL) observed in the reaction of U (IV) with xenon difluoride (XeF_2) results from two reactions occurring in parallel: reduction of XeF_2 with U (IV) and with water. The kinetics of this reaction were investigated. It was shown that CL intensity (I_{CL}) reached a maximum some time after mixing the reagents and not at time zero, after which it dropped off exponentially. The induction period depends on reagent concentration and reaction temperature. The reaction rate following the induction period is of the first order with respect to U (IV). Reaction rate constants obtained by the three methods (chemiluminescence, spectrophotometry, and spectrofluorometry) are similar. It was concluded that the reaction goes through the stage of uranyl ion UO_2^{2+} formation and that the stages of UO_2^{2+} formation and luminescence are superimposable. Oxidation of U (IV) is preceded by formation of the complex $\text{U}^{IV}\text{XeF}_2$ as the initial step after the reagents are mixed, leading to changes in optical density of the solution. Figures 3; references 12: 9 Russian, 3 Western.

7813/9604

Mathematical Modeling and Remote Control of Ion Exchange Processes for Separation of Transplutonium Elements

18410217b Leningrad RADIOKHIMIYA in Russian Vol 29, No 6, Nov-Dec 87 (manuscript received 16 Dec 86) pp 773-776

[Article by I.V. Tselishchev and A.A. Yezesin]

[Abstract] During the process of separating two substances, some values are obtainable at the beginning of the process, while others may have to be obtained during the actual elution from early segments of the elution curve. This may be achieved by a remote process, using rather complex mathematical equations. A mathematical model and an algorithm for calculating elution curves during separation of transplutonium elements (TPE), optimal fractionation limits of the compounds being separated, yield, and the degree of purification were reported. The program was written for the "Elektronika Dz-28" microcomputer. Data from the actual separation of curium and americium as well as einsteinium and californium were found to be in good agreement with those obtained from such algorithms. The calculations could be performed either by preliminary selection of the

conditions or in real time during the process itself. This algorithm could serve in development of an automated control system for the separation process. Figures 2; references 2 (Russian).

7813/9604

Radiochemical Investigation of Hydroxide Films. Part V: Effect of Carbonate Ion on Statics and Kinetics of Uranium Microquantity Sorption on Thin Layer Titanium Hydroxide

18410217c Leningrad RADIOKHIMIYA in Russian Vol 29, No 6, Nov-Dec 87 (manuscript received 22 Dec 86) pp 787-794

[Article by T.A. Nedobukh, V.V. Kafaylov, and N.D. Betenekov]

[Abstract] Hydroxide solvents, including those based on titanium hydroxide, are very effective collectors of uranium from complex sea water-salt solutions. The effect of carbonate ions on uranium behavior is very important because most uranium is found in sea water in the form of its tricarbonat complex. Therefore, this aspect was investigated in this work, showing that increased concentration of carbonates in the solution leads to a lower coefficient of separation because of the formation of nonadsorbing titanium hydroxide of the uranyl tricarbonat complex. The limiting step in uranium sorption is the dissociation of its tricarbonat form; principal kinetic parameters of this process were calculated. It is possible to lower carbonate ion concentration only by special decarbonization methods or by shifting the pH of the solution to 5-5.5, but then uranium converts principally to the uranyl hydroxy form. Figures 6; references 15: 12 Russian, 3 Western (1 by Russian authors).

7813/9604

Use of ^{237}Pu for Chemical Control of Plutonium Yield in Course of Its Isolation from Environmental Samples

18410217d Leningrad RADIOKHIMIYA in Russian Vol 29, No 6, Nov-Dec 87 (manuscript received 18 Jan 87) pp 819-822

[Article by A.D. Gedeonov, L.A. Pelevin, L.P. Bakushkina, and A.N. Suprunenko]

[Abstract] Current methods used in determination of microquantities of plutonium in environmental samples use two labels in estimating the chemical yield: Pu-236 and Pu-242, both of which exclude the possibility of using γ -radiation as a means of registering their activity, and thus are limited in their application. The goal of this study was to evaluate the feasibility of using Pu-237 for this purpose. A specific example of a soil sample from the Leningrad area was described in detail, indicating various purification steps. Final analysis performed by α -spectrophotometric determination of Pu-236 and Pu-238 and in comparison to Pu-237 showed good agreement

within the experimental error. It was shown that Pu-237 could be used to identify stages at which principal losses of plutonium occur; this aspect is very important during development of new technology. Figure 1; references 8: 2 Russian, 6 Western.

7813/9604

Solidification of Aqueous Tritium-Containing Wastes, Using Calcium and Bitumen Oxide
18410217e Leningrad RADIOKHIMIYA in Russian
Vol 29, No 6, Nov-Dec 87 (manuscript received
25 Feb 86) pp 829-834

[Article by V.N. Shchebetovskiy, A.A. Bochkov, and V.I. Skryabin]

[Abstract] A simple method was proposed for solidification of aqueous tritium-containing wastes, using calcium and bitumen oxides. It is based on treating these aqueous

wastes with calcium oxide at a ratio of 1:3.5, obtaining a dry powder of tritiated calcium hydroxide, and adding it to molten bitumen. After solidification of this mixture, water-stable compounds are obtained. The goal of this work was to study isolation of oxidized forms of tritium during contact of $\text{Ca}(\text{OH})(\text{OT})$ with molten bitumen and to investigate resistance of the compounds obtained to leaching-out of tritium and calcium with water. It was shown that the loss of HTO is low, ranging from 0.0014 to 0.0026%; even at 210° C, this loss did not exceed $5.9 \cdot 10^{-4}\%$ of the starting level. In one year, only 1.1% of tritium was lost from bitumen hydroxide blocks, while 38% was lost from cement blocks. From analysis of the data obtained, it was concluded that calcium oxide should be used to solidify aqueous tritium-containing wastes, followed by combining tritiated calcium hydroxide with bitumen. Figures 4; references 6: 5 Russian (3 by Western authors), 1 Western.

7813/9604

**Bis(3-oxa-1,5-dithiapentano)tetrathiafulvalene:
Novel Electron Donor**

18410213b Riga KHIMIYA

*GETEROTSIKLICHESKIKH SOYEDINENIY in
Russian No 11, Nov 87 (manuscript received 19 Jun 86;
in final form 26 Mar 87) pp 1483-1485*

[Article by V.S. Russkikh and G.G. Abashev, Perm State
University imeni A.M. Gorkiy]

[Abstract] A search was conducted for novel compounds having the structural characteristics of bis(ethylenedithio)tetrathiafulvalene, since the latter serves as the basis for "organic metal" superconductors with the highest known critical temperatures among organic compounds. A series of 1,3-dithiol-2-thione (DT) derivatives were synthesized by the reaction of bis(tetrabutylammonium)bis(1,3-dithiol-2-thione-4,5-dithiolato)zincate with selected ethers ($\text{CICH}_2\text{OCH}_2\text{Cl}$, $\text{CICH}_2\text{SH}_2\text{Cl}$, Cl_2CHOH_2 , $\text{Cl}_2\text{CHSCH}_2$) at 50°C in acetone. Of the resultant products — 4,5-(3'-oxa-1',5'-dithiapentano)-DT (I), 4,5-(1',3',5'-trithiapentano)-DT, 4,5-(2'-methoxy-1',3'-dithiapropano)-DT, and 4,5-(2'-methylthio-1',3'-dithiapropano)-DT — reaction of I with mercury acetate led to synthesis of the ketone 4,5-(3'-oxa-1',5'-dithiapentano-1,3-dithiol-2-thione (II). Heating II with triethyl phosphite at $130-140^\circ\text{C}$ under argon led to the synthesis of bis(3-oxa-1,5-dithiapentano)tetrathiafulvalene, a novel electron donor. References 9: 6 Russian, 3 Western.

12172/9604

**Spectroscopy of Electrically Conducting Organic
Ion-Radical Salts. Interaction of Conductivity
Electrons With Molecular Vibrations**

18410219b Moscow KHIMICHESKAYA FIZIKA in
*Russian Vol 6, No 11, Nov 87 (manuscript received
3 Mar 87) pp 1529-1548*

[Article by M.G. Kaplunov and Yu.G. Borodko, Insti-
tute of Chemical Physics, Chernogolovka Branch, USSR
Academy of Sciences]

[Abstract] Organic conductors such as ion-radical salts (IRS) and conducting polymers are studied widely because of their interesting electrophysical properties, especially in the area of high temperature superconductivity. Optical properties of conducting IRSs were reviewed, especially interactions of IR vibrations with conducting electrons (excitation of these vibrations with charge transfer). The following compounds were covered, reviewing parameters such as electronic transfer integrals and electronic-vibrational interaction constants: potassium cyanoplatinate, tetracyanoquinodimethane, tetrathiotetracene, tetraselenotetracene, tetrathiafulvalene, tetraselenafulvalene, tetramethyltetrathiafulvalene, tetramethyltetraselenafulvalene, dibenzotetrathiafulvalene, bis(ethylenedithio)tetrathiafulvalene, hexamethylenetetraselenafulvalene,

tetracyanonaphtaquinodimethane, triethylammonium, methyltriphenylphosphonium, methylethylmorpholinium, ditoluolchromium, trimethylammonium, trimethylbenzimidazolium, dimethylbenzimidazolium, decamethylferrocene, and N-methyl-2,6-dimethylpyridine. Figures 6; references 137: 37 Russian (2 by Western authors), 100 Western (13 by Russian authors).

7813/9604

**Development of Automatic Data Bank for
Physicochemical Gas Dynamics**

18410228b Moscow KHIMICHESKAYA FIZIKA

*in Russian Vol 6, No 12, Dec 87 (manuscript received
28 Apr 87) pp 1677-1695*

[Article by S.A. Losev and O.P. Shatalov, Institute of
Mechanics, Moscow State University imeni M.V. Lomo-
nosov]

[Abstract] A discussion is presented of some of the problems that are encountered in establishing a computerized data bank for physicochemical gas dynamics and the methods to be employed to ensure their currency. The fundamental problems pertain to the fact that, concerning thermodynamic data, physicochemical kinetic information is not universal but dependent on ambient conditions and outside influences. Thus, the accuracy of a computerized data bank depends on constantly updating and introducing new data, both according to numerical and model-based parameters. The essential process involves intellectualization of computers to secure their optimum validity as data storage and processing devices with regard to ever-changing information. These considerations led to the development of the AVOGADRO system for automatic substantiation of recommendations for gas dynamics and evaluation of data reliability. The system, as currently formulated, encompasses four components represented by a bank of physicochemical data and their models, a generator of reaction medium models, a library of programmable modules, and a constructor of program combinations. The system was found efficient when applied to gases and their components in relatively simple systems at thermal energies. Figures 9; tables 4; references 73: 26 Russian, 47 Western.

12172/9604

**Molecular Design and Computers. Part 10.
Recalculation and Generation of Equations for
Ionic, Radical, and Redox Processes With Linear
Electron Transfer**

18410229a Leningrad ZHURNAL ORGANICHESKOY
KHIMII in Russian Vol 23, No 12, Dec 87 (manuscript
received 31 Jul 86) pp 2488-2507

[Article by S.S. Trach, G.A. Gamziani and N.S. Zefirov,
Moscow State University imeni M.V. Lomonosov]

[Abstract] A review is provided of the recent advances in mathematical modeling of multicentric chemical processes involving linear electron transfer, based on symbolic equations describing ionic and radical reactions.

These systems involve noncanonical linear bond redistributions with a single mode, with the symbolic equations being derived from equations describing reactions with cyclic electron transfer [Zefirov, NS et al., Zhurn. Org. Khim., 22(7): 1341, 1986]. The symbolic equations describing linear electron transfer processes are accomplished by replacing univalent reaction centers in the equations applicable to cyclic electron transfer with symbols representing charge or an unpaired electron, i.e., (+), (-), and (\cdot). Since formalized mathematical generation of symbolic equations for linear electron transfer processes employs discrete mathematics, it represents, in

many respects, a straightforward approach to molecular design. A method was developed for direct generation of a complete description of such processes, utilizing Burnside's lemma, with the algorithm written in BASIC version 02 designed for the Iskra-226.6 microcomputer. The complete text of the program and its applications will be published separately and deposited with VINITI in the "Algorithms and Programs for Computerized Molecular Design" series. References 21: 18 Russian, 3 Western.

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